

*Office of Technical Assistance Research Proposal*  
***Statistical Mechanical Usage in “Green” Chemistry***

**BACKGROUND**

At a recent conference on “Green Chemistry” the proposal was raised to explore the use of quantum mechanical methods in characterizing new polymers. This was immediately rejected due to the fact that quantum mechanics cannot be used for this application for chain lengths greater than three molecules. An alternate approach to gaining an understanding of large macromolecules is to apply statistical mechanical methods in the manner of Flory (1). While less accurate, these methods can lead to mathematical expressions of these molecules for solubility, glass transition temperature, melting point etc.

With the description of a particular macromolecule, the method of synthesis may be apparent. Since the manufacturing process will be a significant source of environmental pollution related to a polymer, the synthesis route used to produce new polymers will largely determine their “Greenness”. Consequently, mathematical expressions derived from statistical mechanical methods could allow for polymers to be quickly screened for suitability of synthesis.

The manufacturing of greener polymers would be anticipated to reduce the use of TURA-regulated chemicals by Massachusetts manufacturers of plastics materials and resins (SIC code 2821). For example, in 1998, 345 million lbs. of styrene, 3.9 million lbs. of butyl acrylate, 7.9 million lbs. of methyl methacrylate, and 2 million lbs. of ethyl acrylate were reported under TURA. Some of the largest users of these chemicals were companies such as Polymer Latex, Interpolymer Corp., Zeneca Resins, and Novacor Chemical.

**SCOPE OF PROBLEM**

The elimination of plastics with an adverse impact on the environment either in production or disposal will be a formidable task. While we should not expect immediate results the job should be started.

**PROGRAM OBJECTIVE**

The basic objective will be to develop those mathematical techniques needed to formulate the various thermodynamic expressions to define the new polymers.

**SCOPE OF WORK**

Initially it will be necessary to identify suitable candidate polymers based on atomic content and to develop statistical thermodynamic models as a basis for future exploration.

OTA can assist in the identification of an industry partner.

1) For instance see: “Configurational Statistics of Polymer Chains”, M.V. Volkenstein  
Interscience Publishers, 1963, New York